1-Butanol, 3-methoxy-3-methyl-, acetate 103429-90-9 | DTXSID30145852

103429-9	10-9 D	1 X 2 1 D 3 0	1145852

Model Performance

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Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 6.02e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.04e-01

Confidence level: 7.02e-01

Nearest Neighbors from the Training Set

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Butyl 3-methoxypropionate Measured: 6.12e-02 Predicted: 6.04e-02

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2-Butoxyethyl acetate Measured: 5.62e-02 Predicted: 6.06e-02

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Methyl 3-butoxypropanoate Measured: 5.12e-02 Predicted: 5.88e-02

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propyl 3-propoxypropanoate

Measured: 2.07e-02 Predicted: 3.66e-02